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(56) Documents cited by ISA
US 5025388 A US 4642762 A US 4473889 A
US 4461619 A

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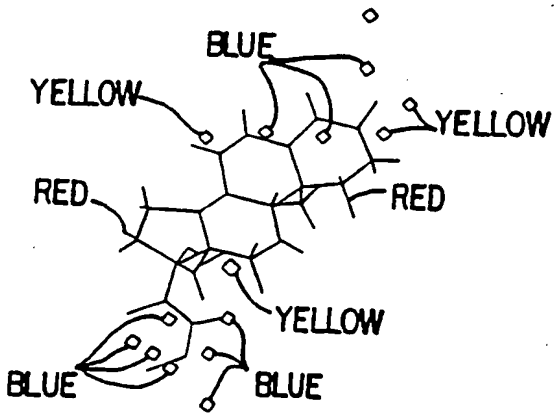
(54) Comparative molecular field analysis (CoMFA)

(57) Comparative Molecular Field Analysis (CoMFA) is an effective computer implemented methodology (Fig. 5) of 3D-QSAR employing both interactive graphics and statistical techniques for correlating shapes of molecules with their observed biological properties. For each molecule of a series of known substrates the steric and electrostatic interaction energies with a test probe atom are calculated at spatial coordinates around the molecule. Subsequent analysis of the data table by a partial least squares (PLS) cross-validation technique (Fig. 8) yields a set of coefficients which reflect the relative contribution of the shape elements of the molecular series to differences in biological activities. Display (Fig. 3B) in three dimensions in an interactive graphics environment of the spatial volumes highly associated with biological activity and comparison with molecular structures yields an understanding of intermolecular associations. CoFMA will also predict the biological activity of new molecular species.



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